16. Adsorption to a surface  

Consider a solid surface to be a two-dimensional lattice with $M$ sites. Each site can be either empty or occupied with a single adsorbed atom. An adsorbed atom has a binding energy $-\varepsilon$ and we neglect any interactions between the atoms.

a) Calculate the grand canonical partition function of the adsorbed atoms as a function of temperature $T$, lattice size $M$, and chemical potential $\mu'$. Use variables $n_i \in \{0, 1\}$ for each $i = 1, \ldots, M$ to describe if site $i$ is empty or occupied.

b) Calculate the grand canonical potential of the adsorbed atoms as a function of temperature $T$, lattice size $M$, and chemical potential $\mu'$.

c) Calculate the average number of adsorbed atoms $N$ as a function of temperature $T$, lattice size $M$, and chemical potential $\mu'$.

d) The surface is exposed to an ideal gas of the atoms at some pressure $P$ and the same temperature $T$ as the surface. Calculate the fraction $N/M$ of adsorbed atoms as a function of the pressure $P$ of the ideal gas and the temperature $T$ of the system. (Hint: in thermodynamic equilibrium the chemical potentials of the adsorbed atoms and the atoms in the ideal gas have to be equal.)

17. Density operator  

a) In a two-dimensional Hilbert space an operator $\hat{\rho}$ is given by the matrix

$$
\hat{\rho} = \frac{1}{2} \begin{pmatrix}
1 + a_1 & a_2 \\
 a_3 & 1 - a_1
\end{pmatrix}.
$$

Determine for which values of the three complex parameters $a_1$, $a_2$, and $a_3$ this operator is a density operator. For which values of the three parameters is it a pure state?

b) Prove that for a hermitian Hamiltonian $\hat{H}$ the operator $\hat{\rho} \equiv e^{-\beta \hat{H}}/\text{tr} e^{-\beta \hat{H}}$ is a density operator.